Author Index to Volume 156

Adamowicz, L., Theoretical study of optical excitations of linear C_4^- 156 (1991) 387

Bagchi, B., see A. Chandra 156 (1991) 323
Bahatt, D., U. Even, E. Shalev, N. Ben-Horin and J. Jortner, Isomer-specific radiative lifetimes of molecular heteroclusters 156 (1991) 223
Baldeck, P.L., see M. Pierre 156 (1991) 103
Bañares, L., see A. Heikal 156 (1991) 231
Banerjee, A.K., see T. Kundu 156 (1991) 95
Bednarek, G., see J. Wildt 156 (1991) 497
Benetis, N.P., see L. Sjöqvist 156 (1991) 457
Ben-Horin, N., see D. Bahatt 156 (1991) 223
Besnainou, S., G. Cardini and D.A. Dows, Molecular dynamics simulation of crystalline imidazole 156 (1991) 71
Bitto, H., see P.R. Willmott 156 (1991) 177
Blinc, R., see E. Hadjoudis 156 (1991) 149
Block, D., see M. Pierre 156 (1991) 103
Bohr, F. and M.F. Ruiz-López, Theoretical study of multiple-scattering effects in the X-ray absorption spectra of iron-porphyrins 156 (1991) 55
Braga, M., A. Broo and S. Larsson, Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers 156 (1991) 1
Brock, L., see T. Devore 156 (1991) 156
Broo, A., see M. Braga 156 (1991) 1
Brühlmann, U., see M. Lombardi 156 (1991) 163

Cardini, G., see S. Besnainou 156 (1991) 71
Češpiva, L., see J. Vojtík 156 (1991) 369
Chaiyapongs, S., see K.P. Sagarik 156 (1991) 439
Champagne, B.B., D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts, The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states 156 (1991) 251
Chandra, A. and B. Bagchi, Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid 156 (1991) 323
Chapoulard, D., see S. Guizard 156 (1991) 509
Choo, K.Y., see S. Lee 156 (1991) 339
Chowdhury, M., see T. Kundu 156 (1991) 95
Colpa, J.P. and F.P. Temme, Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)^1\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)^1\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110. Erratum 156 (1991) 532
Crépin, C. and A. Tramer, Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices 156 (1991) 281

Cuadros, F. and A. Mulero, Scaling the WCA reference system for two-dimensional Lennard-Jones fluids 156 (1991) 33

Decleva, P., see M. Ohno 156 (1991) 309
De Lange, P.J., see B.R. Veenstra 156 (1991) 157
De Lange, P.J., H.Th. Jonkman and K.E. Drabe, Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine 156 (1991) 209
Devore, T., L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole, On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433. Erratum 156 (1991) 156
Dezarnaud, C., M. Tronc and A. Modelli, Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2 156 (1991) 129
Domcke, W., see A. Staib 156 (1991) 21
Dovesi, R., C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders, On the elastic properties of lithium, sodium and potassium oxide. An ab initio study 156 (1991) 11
Dows, D.A., see S. Besnainou 156 (1991) 71
Drabe, K.E., see P.J. de Lange 156 (1991) 209
Dulaney, K., see T. Devore 156 (1991) 156

Eggenberger, R., S. Gerber, H. Huber and D. Searles, Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2 156 (1991) 395
Engeln, R. and J. Reuss, Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2 156 (1991) 215
Even, U., see D. Bahatt 156 (1991) 223

Faegri Jr., K., see O. Swang 156 (1991) 379
Fink, E.H., see J. Wildt 156 (1991) 497
Fraser, G.T., A.S. Pine, W.A. Kreiner and R.D. Suenram, Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3 156 (1991) 523
Freyria-Fava, C., see R. Dovesi 156 (1991) 11

Gauyacq, D., see S. Guizard 156 (1991) 509
Georges, R., see M. Pierre 156 (1991) 103
Gerber, S., see R. Eggenberger 156 (1991) 395
Gole, J.L., see T. Devore 156 (1991) 156
Gropen, O., see O. Swang 156 (1991) 379
Guizard, S., N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq, Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO 156 (1991) 509
Gülen, D., Fluorescence depolarization in nonlinear molecular pairs 156 (1991) 123
Gutsev, G.L., The structure and stability of Cl_n^- clusters, $n=2$–7 156 (1991) 427

Hadjoudis, E., F. Milia, J. Seliger, V. Zagar and R. Blinc, ^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds 156 (1991) 149
Heikal, A., L. Bañares, D.H. Semmes and A.H. Zewail, Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$) 156 (1991) 231
Heydtmann, H., see C. Kaupert 156 (1991) 85
Horani, M., see S. Guizard 156 (1991) 509

Huber, H., see R. Eggenberger 156 (1991) 395
Huber, J.R., see M. Lombardi 156 (1991) 163
Huber, J.R., see P.R. Willmott 156 (1991) 177

Ida, T., K. Yakushi, H. Kuroda, H. Yamochi and G. Saito, Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD) 156 (1991) 113

Jonkman, H.Th., see P.J. de Lange 156 (1991) 209
Jortner, J., see D. Bahatt 156 (1991) 223

Kahlscheuer, R., see T. Devore 156 (1991) 156
Kaupert, C., H. Heydtmann and W. Thiel, The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane 156 (1991) 85
Kokpol, S., see Y.P. Yongyai 156 (1991) 403
Kommandeur, J., see B.R. Veenstra 156 (1991) 157
Kreiner, W.A., see G.T. Fraser 156 (1991) 523
Kroes, G.-J. and R.P.H. Rettschnick, Vibrational relaxation of glyoxal in collisions with He and Ar 156 (1991) 293
Kundu, T., A.K. Banerjee and M. Chowdhury, Circular dichroism spectrum of gadolinium diglycolate single crystal 156 (1991) 95
Kuroda, H., see T. Ida 156 (1991) 113

Larsson, S., see M. Braga 156 (1991) 1
Lee, D., see S. Lee 156 (1991) 339
Lee, S., M. Yang, K.J. Shin, K.Y. Choo and D. Lee, Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity 156 (1991) 339
Lombardi, M., J.P. Pique, U. Brühlmann and J.R. Huber, S_1–T_1 coupling in propynal by level anticrossing spectroscopy 156 (1991) 163
Lund, A., see L. Sjöqvist 156 (1991) 457

Mai, J. and W. von Niessen, The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$ 156 (1991) 63
Maruani, J., see L. Sjöqvist 156 (1991) 457
Meerts, W.L., see P. Uijt de Haag 156 (1991) 197
Meerts, W.L., see B.B. Champagne 156 (1991) 251
Meijers, H.C., see B.R. Veenstra 156 (1991) 157
Milia, F., see E. Hadjoudis 156 (1991) 149
Modelli, A., see C. Dezarnaud 156 (1991) 129
Mulero, A., see F. Cuadros 156 (1991) 33

Nakashima, K., see T. Ogawa 156 (1991) 465
Nakashima, K., see T. Ogawa 156 (1991) 473

O, H.-K., see M.-C. Su 156 (1991) 261
Ogawa, T., T. Tsuboi and K. Nakashima, Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom 156 (1991) 465

Ogawa, T., M. Tsukada and K. Nakashima, Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$ 156 (1991) 473
Ohno, M. and P. Decleva, Many-body calculations of the core hole spectra of NiCO 156 (1991) 309

Paidarová, I., see J. Vojtík 156 (1991) 369
Parmenter, C.S., see M.-C. Su 156 (1991) 261
Pfanstiel, J.F., see B.B. Champagne 156 (1991) 251
Pierre, M., P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss, Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals 156 (1991) 103
Pine, A.S., see G.T. Fraser 156 (1991) 523
Pique, J.P., see M. Lombardi 156 (1991) 163
Plusquellic, D.F., see B.B. Champagne 156 (1991) 251
Pongpituk, V., see K.P. Sagarik 156 (1991) 439
Pratt, D.W., see B.B. Champagne 156 (1991) 251
Prencipe, M., see R. Dovesi 156 (1991) 11

Rettschnick, R.P.H., see G.-J. Kroes 156 (1991) 293
Reuss, J., see R. Engeln 156 (1991) 215
Rode, B.M., see Y.P. Yongyai 156 (1991) 403
Roetti, C., see R. Dovesi 156 (1991) 11
Ruiz-López, M.F., see F. Bohr 156 (1991) 55

Sagarik, K.P., V. Pongpituk, S. Chaiyapongs and P. Sisot, Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine 156 (1991) 439
Saito, G., see T. Ida 156 (1991) 113
Saunders, V.R., see R. Dovesi 156 (1991) 11
Šavrda, J., see J. Vojtík 156 (1991) 369
Schleipen, J. and J.J. ter Meulen, State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2 156 (1991) 479
Schulze, K.D., Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism 156 (1991) 43
Searles, D., see R. Eggenberger 156 (1991) 395
Seliger, J., see E. Hadjoudis 156 (1991) 149
Semmes, D.H., see A. Heikal 156 (1991) 231
Shafizadeh, N., see S. Guizard 156 (1991) 509
Shalabi, A.S., Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries 156 (1991) 359
Shalev, E., see D. Bahatt 156 (1991) 223
Shin, K.J., see S. Lee 156 (1991) 339
Siegbahn, P., see O. Swang 156 (1991) 379
Sisot, P., see K.P. Sagarik 156 (1991) 439
Sjöqvist, L., N.P. Benetis, A. Lund and J. Maruani, Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes 156 (1991) 457
Sobolewski, A.L., see A. Staib 156 (1991) 21
Staib, A., W. Domcke and A.L. Sobolewski, Vibronic coupling in Rydberg series of linear molecules 156 (1991) 21

Su, M.-C., H.-K. O and C.S. Parmenter, A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies 156 (1991) 261
Suenram, R.D., see G.T. Fraser 156 (1991) 523
Suzuki, T., see A. Tachibana 156 (1991) 79
Swang, O., K. Faegri Jr., O. Gropen, U. Wahlgren and P. Siegbahn, A theoretical study of the chemisorption of methane on a Ni(100) surface 156 (1991) 379

Tachibana, A., T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe, New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3 \rightarrow NH_2+NH_4^+$ 156 (1991) 79
Tague Jr., T.J. and C.A. Wight, Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine 156 (1991) 141
Tang, K.T. and J.P. Toennies, A combining rule calculation of the van der Waals potentials of the rare-gas hydrides 156 (1991) 413
Temme, F.P., see J.P. Colpa 156 (1991) 532
Teramoto, Y., see A. Tachibana 156 (1991) 79
Ter Meulen, J.J., see J. Schleipen 156 (1991) 479
Thiel, W., see C. Kaupert 156 (1991) 85
Toennies, J.P., see K.T. Tang 156 (1991) 413
Tramer, A., see C. Crépin 156 (1991) 281
Trommsdorff, H.P., see M. Pierre 156 (1991) 103
Tronc, M., see C. Dezarnaud 156 (1991) 129
Tsuboi, T., see T. Ogawa 156 (1991) 465
Tsukada, M., see T. Ogawa 156 (1991) 473

Uijt de Haag, P. and W.L. Meerts, Vibrational and rotational effects on the intersystem crossing in pyrazine and pyrimidine 156 (1991) 197

Van Herpen, W.M., see B.B. Champagne 156 (1991) 251
Veenstra, B.R., H.C. Meijers, P.J. de Lange and J. Kommandeur, The structure of mixed watery clusters 156 (1991) 157
Vojtík, J., L. Češpiva, I. Paidarová and J. Šavrda, Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X\,^2\Sigma^+$ and $B'\,^2\Sigma^+$ states 156 (1991) 369
Von Niessen, W., see J. Mai 156 (1991) 63

Wahlgren, U., see O. Swang 156 (1991) 379
Wayne, R.P., see J. Wildt 156 (1991) 497
Wight, C.A., see T.J. Tague Jr. 156 (1991) 141
Wildt, J., G. Bednarek, E.H. Fink and R.P. Wayne, Laser excitation of the $A\,^3\Sigma_u^+$, $A'\,^3\Delta_u$ and $c\,^1\Sigma_u^-$ states of molecular oxygen 156 (1991) 497
Willmott, P.R., H. Bitto and J.R. Huber, Energy and rotational state dependence of radiationless processes in propynal 156 (1991) 177

Yakushi, K., see T. Ida 156 (1991) 113
Yamabe, T., see A. Tachibana 156 (1991) 79
Yamochi, H., see T. Ida 156 (1991) 113
Yang, M., see S. Lee 156 (1991) 339

Yongyai, Y.P., S. Kokpol and B.M. Rode, Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation 156 (1991) 403
Yoshida, N., see A. Tachibana 156 (1991) 79

Zagar, V., see E. Hadjoudis 156 (1991) 149
Zewail, A.H., see A. Heikal 156 (1991) 231
Zyss, J., see M. Pierre 156 (1991) 103

List of Subjects

1 Methods

1.1 Theoretical

1.1.1 Group theory and algebras *
1.1.2 Classical mechanics *
1.1.3 Quantized field theory
1.1.4 Many body and quasiparticle approaches *
1.1.5 Coupling schemes and perturbative treatments *
1.1.6 Relativistic quantum mechanics
1.1.7 Transport quantum mechanics
1.1.8 Equilibrium statistical mechanics *
1.1.9 Statistical mechanics of stationary states
1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories *
1.1.11 Ab initio schemes for stationary properties *
1.1.12 Computational and simulation methods *
1.1.13 Molecular dynamics and scattering theory *

1.2 Experimental

1.2.1 Magnetic resonances *
1.2.2 Cyclotron resonance
1.2.3 Microwave spectroscopy *
1.2.4 Infrared spectroscopy *
1.2.5 Raman spectroscopy *
1.2.6 Visible and UV spectroscopy *
1.2.7 Fluorescence spectroscopy *
1.2.8 Photoelectron and Auger spectroscopy
1.2.9 X-ray spectroscopy *
1.2.10 Electron impact spectroscopy *
1.2.11 Laser methods *
1.2.12 Picosecond spectroscopy *
1.2.13 Non-linear optical spectroscopy
1.2.14 Synchrotron spectroscopies *
1.2.15 Coherent optical spectroscopy
1.2.16 Optical pumping *
1.2.17 Multiple resonance spectroscopy *
1.2.18 Optoacoustic spectroscopy
1.2.19 Atomic and molecular beam techniques *
1.2.20 Time-resolved experiments *
1.2.21 Mass spectrometry *
1.2.22 Radiolysis
1.2.23 Mössbauer spectroscopy
1.2.24 X-ray, electron and neutron diffraction
1.2.25 Neutron scattering
1.2.26 Light scattering
1.2.27 Field emission and field ionization
1.2.28 Measurement of macroscopic variables

2 Objects

2.1 Bulk systems

2.1.1 Gases *
2.1.2 Supersonic beams *
2.1.3 Liquids neat *
2.1.4 Liquid mixtures and solutions *
2.1.5 Crystals *
2.1.5.1 neat *
2.1.5.2 mixed *
2.1.6 Glasses *
2.1.7 Liquid crystals
2.1.8 Polymers
2.1.9 Semiconductors
2.1.10 Metals and alloys
2.1.11 Thin films
2.1.12 Surfaces *
2.1.13 Low-dimensional materials *
2.1.14 Dielectrics
2.1.15 Plasmas
2.1.16 Biological systems *

2.2 Microscopic systems

2.2.1 Atoms
2.2.2 Molecules (neutral and ionic) *
2.2.2.1 diatomic *
2.2.2.2 small polyatomics *
2.2.2.3 aromatics *
2.2.2.4 other large *
2.2.2.5 polymeric and biological *
2.2.3 Molecular aggregates *
2.2.3.1 dimers *
2.2.3.2 van der Waals molecules *
2.2.3.3 clusters *
2.2.3.4 complexes *
2.2.4 Free radicals (including hydronium and muonium) *
2.2.5 Quasiparticles (including excitons) *
2.2.6 Defects and impurities
2.2.7 Ions and charge carriers *

* Denotes subjects covered in this volume

3 Phenomena

3.1 Molecular structure *
3.2 Vibrations and rotations of molecules *
3.3 Electronic structure and states *
3.4 Electric and magnetic properties
3.5 Spin splittings *
3.6 Optical activity
3.7 Molecular interactions *
3.8 Spectral bandshapes and intensities *
3.9 Coupling of electronic and nuclear motion *
3.10 Energy transfer processes *
3.11 Molecular photophysical processes *
3.12 Intramolecular dynamics *
3.12.1 radiationless transitions *
3.12.2 vibrational energy redistribution (including vibrational dissociation)
3.13 Luminescence spectra, yields and lifetimes *
3.14 Coherence loss processes
3.15 Non-linear responses (including optical) *
3.16 Multiphoton phenomena *
3.17 Reactions (including dissociation) *
3.17.1 gas phase *
3.17.2 condensed phase *
3.17.3 photochemical
3.18 Tunnelling
3.19 Electron transfer *
3.20 Positron annihilation
3.21 Ionization (including Rydberg states) *
3.22 Molecular motion (including diffusive) *
3.23 Isotopic effects
3.24 Fluctuations and noise
3.25 Collective motion and excitations *
3.26 Surface effects and catalysis *
3.27 Thermodynamic and transport properties *
3.28 Structure of solids and liquids *
3.29 Critical phenomena *
3.30 Phase transitions *

Subject Index to Volume 156

Methods

Theoretical

Group theory and algebras

Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)^1\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)^1\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110., J.P. Colpa and F.P. Temme 156 (1991) 532

Classical mechanics

New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3 \rightarrow NH_2+NH_4^+$. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79

Many body and quasiparticle approaches

Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359

Coupling schemes and perturbative treatments

Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21
Scaling the WCA reference system for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 156 (1991) 33

Equilibrium statistical mechanics

Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation, Y.P. Yongyai, S. Kokpol and B.M. Rode 156 (1991) 403

Non-equilibrium thermodynamic and hydrodynamic theories

Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid, A. Chandra and B. Bagchi 156 (1991) 323
Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339

Ab initio schemes for stationary properties

Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1
On the elastic properties of lithium, sodium and potassium oxide. An ab initio study, R. Dovesi, C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders 156 (1991) 11

The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane, C. Kaupert, H. Heydtmann and W. Thiel 156 (1991) 85
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X\,^2\Sigma^+$ and $B'\,^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369
A theoretical study of the chemisorption of methane on a Ni(100) surface, O. Swang, K. Faegri Jr., O. Gropen, U. Wahlgren and P. Siegbahn 156 (1991) 379
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2, R. Eggenberger, S. Gerber, H. Huber and D. Searles 156 (1991) 395
The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427

Computational and simulation methods
On the elastic properties of lithium, sodium and potassium oxide. An ab initio study, R. Dovesi, C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders 156 (1991) 11
Scaling the WCA reference system for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 156 (1991) 33
Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism, K.D. Schulze 156 (1991) 43
Theoretical study of multiple-scattering effects in the X-ray absorption spectra of iron-porphyrins, F. Bohr and M.F. Ruiz-López 156 (1991) 55
The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71
Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2, R. Eggenberger, S. Gerber, H. Huber and D. Searles 156 (1991) 395
Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation, Y.P. Yongyai, S. Kokpol and B.M. Rode 156 (1991) 403
A combining rule calculation of the van der Waals potentials of the rare-gas hydrides, K.T. Tang and J.P. Toennies 156 (1991) 413
The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427
Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457

Molecular dynamics and scattering theory
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71

New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v) + NH_3 \rightarrow NH_2 + NH_4^+$. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79
Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
A combining rule calculation of the van der Waals potentials of the rare-gas hydrides, K.T. Tang and J.P. Toennies 156 (1991) 413

Experimental

Magnetic resonances

^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457
Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)^1\mathcal{G}$ symmetries. II. $\Gamma/\bar{\Gamma}$ $(\mathcal{S}_6)^1\mathcal{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110., J.P. Colpa and F.P. Temme 156 (1991) 532

Microwave spectroscopy

Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523

Infrared spectroscopy

The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane, C. Kaupert, H. Heydtmann and W. Thiel 156 (1991) 85
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523

Raman spectroscopy

Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2, R. Engeln and J. Reuss 156 (1991) 215

Visible and UV spectroscopy

Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433., T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156

Vibrational and rotational effects on the intersystem crossing in pyrazine and pyrimidine, P. Uijt de Haag and W.L. Meerts 156 (1991) 197
Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209
The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251
Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281

Fluorescence spectroscopy
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281

X-ray spectroscopy
Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129

Electron impact spectroscopy
Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129
Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465
Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473

Laser methods
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
S_1–T_1 coupling in propynal by level anticrossing spectroscopy, M. Lombardi, J.P. Pique, U. Brühlmann and J.R. Huber 156 (1991) 163
Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223
Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479
Laser excitation of the $A^3\Sigma_u^+$, $A'^3\Delta_u$ and $c^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497

Picosecond spectroscopy
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123

Real-time dynamics of vibrational predissociation in anthracene–Ar_n (n=1,2,3), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231

Synchrotron spectroscopies

Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129

Optical pumping

Laser excitation of the $A^3\Sigma_u^+$, $A'^3\Delta_u$ and $c^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497

Multiple resonance spectroscopy

Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509

Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)^1\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)^1\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110., J.P. Colpa and F.P. Temme 156 (1991) 532

Atomic and molecular beam techniques

On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433., T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156

The structure of mixed watery clusters, B.R. Veenstra, H.C. Meijers, P.J. de Lange and J. Kommandeur 156 (1991) 157

S_1–T_1 coupling in propynal by level anticrossing spectroscopy, M. Lombardi, J.P. Pique, U. Brühlmann and J.R. Huber 156 (1991) 163

Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465

Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473

State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479

Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523

Time-resolved experiments

Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177

Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209

Mass spectrometry

The structure of mixed watery clusters, B.R. Veenstra, H.C. Meijers, P.J. de Lange and J. Kommandeur 156 (1991) 157

The structure and stability of Cl_n^- clusters, n=2–7, G.L. Gutsev 156 (1991) 427

Objects

Bulk systems

Gases

Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129
Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2, R. Engeln and J. Reuss 156 (1991) 215
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2, R. Eggenberger, S. Gerber, H. Huber and D. Searles 156 (1991) 395
Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509

Supersonic beams

The structure of mixed watery clusters, B.R. Veenstra, H.C. Meijers, P.J. de Lange and J. Kommandeur 156 (1991) 157
Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177
Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479

Liquids neat

Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid, A. Chandra and B. Bagchi 156 (1991) 323

Liquid mixtures and solutions

Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339
Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation, Y.P. Yongyai, S. Kokpol and B.M. Rode 156 (1991) 403

Crystals

On the elastic properties of lithium, sodium and potassium oxide. An ab initio study, R. Dovesi, C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders 156 (1991) 11
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71
^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359

–neat
Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103

–mixed
Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281

Glasses
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141

Surfaces
The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63
A theoretical study of the chemisorption of methane on a Ni(100) surface, O. Swang, K. Faegri Jr., O. Gropen, U. Wahlgren and P. Siegbahn 156 (1991) 379

Low-dimensional materials
Scaling the WCA reference system for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 156 (1991) 33
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113

Biological systems
Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism, K.D. Schulze 156 (1991) 43
Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439

Microscopic systems

Molecules (neutral and ionic)
New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3 \rightarrow NH_2+NH_4^+$, A. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79
^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457

Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523

–diatomic

On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433., T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156

Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X^2\Sigma^+$ and $B'^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369

A combining rule calculation of the van der Waals potentials of the rare-gas hydrides, K.T. Tang and J.P. Toennies 156 (1991) 413

Laser excitation of the $A^3\Sigma_u^+$, $A'^3\Delta_u$ and $c^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497

Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509

–small polyatomics

Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21

The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane, C. Kaupert, H. Heydtmann and W. Thiel 156 (1991) 85

S_1–T_1 coupling in propynal by level anticrossing spectroscopy, M. Lombardi, J.P. Pique, U. Brühlmann and J.R. Huber 156 (1991) 163

Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177

Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209

Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2, R. Engeln and J. Reuss 156 (1991) 215

Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465

Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473

–aromatics

The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251

–other large

Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1

Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95

Vibrational and rotational effects on the intersystem crossing in pyrazine and pyrimidine, P. Uijt de Haag and W.L. Meerts 156 (1991) 197

Structure of MQ-NMR spin spaces under higher $\mathcal{S}_n$- and $(\mathcal{S}_n)^1\mathcal{G}$ symmetries. II. $\Gamma/\bar{\Gamma}$ $(\mathcal{S}_6)^1\mathcal{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110., J.P. Colpa and F.P. Temme 156 (1991) 532

–polymeric and biological
Theoretical study of multiple-scattering effects in the X-ray absorption spectra of iron-porphyrins, F. Bohr and M.F. Ruiz-López 156 (1991) 55

Molecular aggregates
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113
Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439

–dimers
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123
Ab initio calculation of the second virial coefficient of neon and the potential energy curve of Ne_2, R. Eggenberger, S. Gerber, H. Huber and D. Searles 156 (1991) 395

–van der Waals molecules
The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
A combining rule calculation of the van der Waals potentials of the rare-gas hydrides, K.T. Tang and J.P. Toennies 156 (1991) 413

–clusters
The structure of mixed watery clusters, B.R. Veenstra, H.C. Meijers, P.J. de Lange and J. Kommandeur 156 (1991) 157
Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223
Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281
Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427

–complexes
Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95

Free radicals (including hydronium and muonium)
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457

Quasiparticles (including excitons)
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123

Ions and charge carriers
Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387

Phenomena

Molecular structure
^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433., T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156
The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
Nodal configurations and many-body energies in Li_3^{3+}, F_3^{3-}, $Li_2^{2+}F^-$ and $Li^+F_2^{2-}$ ions at crystal and cluster geometries, A.S. Shalabi 156 (1991) 359
Test-particle model potentials for hydrogen-bonded complexes: complexes formed from HCN, HF, H_2O, NH_3, $HCONH_2$, $HCONHCH_3$, guanine and cytosine, K.P. Sagarik, V. Pongpituk, S. Chaiyapongs and P. Sisot 156 (1991) 439

Vibrations and rotations of molecules
The vibrational spectra of the monohalogenated cyclopropanes: ab initio calculations and an experimental study of fluorocyclopropane, C. Kaupert, H. Heydtmann and W. Thiel 156 (1991) 85
Methyl torsion in $C_2H_{4-n}(CH_3)_n$, $n=1$ or 2, R. Engeln and J. Reuss 156 (1991) 215
A fluorescence characterization of the *p*-difluorobenzene–argon van der Waals complex. Energy levels, geometries and dissociation energies, M.-C. Su, H.-K. O and C.S. Parmenter 156 (1991) 261
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X^2\Sigma^+$ and $B'^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369

Electronic structure and states
Circular dichroism spectrum of gadolinium diglycolate single crystal, T. Kundu, A.K. Banerjee and M. Chowdhury 156 (1991) 95
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103

Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113
Shape resonances in low-energy electron transmission and sulfur K-shell photoabsorption spectroscopies: CH_3SH, C_2H_5SH, $(CH_3)_2S$, $(C_2H_5)_2S$, C_6H_5SH, $C_6H_5SCH_3$, CH_3SCN, CH_3NCS, SCl_2, C. Dezarnaud, M. Tronc and A. Modelli 156 (1991) 129
^{14}N NQR investigation of some thermochromic and photochromic salicylideneanilines and related compounds, E. Hadjoudis, F. Milia, J. Seliger, V. Zagar and R. Blinc 156 (1991) 149
On the BiF bond dissociation energy and an evaluation of the BiF red emission band systems, Chem. Phys. 155 (1991) 423–433., T. Devore, L. Brock, R. Kahlscheuer, K. Dulaney and J.L. Gole 156 (1991) 156
Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209
Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X^2\Sigma^+$ and $B'^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369
The structure and stability of Cl_n^- clusters, $n=2$–7, G.L. Gutsev 156 (1991) 427
Laser excitation of the $A^3\Sigma_u^+$, $A'^3\Delta_u$ and $c^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497

Spin splittings
Nuclear quadrupole coupling constants of rovibrational levels of all isotopic species of BH^+ in their $X^2\Sigma^+$ and $B'^2\Sigma^+$ states, J. Vojtík, L. Češpiva, I. Paidarová and J. Šavrda 156 (1991) 369
Structure of MQ-NMR spin spaces under higher $\mathscr{S}_n$- and $(\mathscr{S}_n)^{\downarrow}\mathscr{G}$ symmetries. II. $\Gamma/\tilde{\Gamma}$ $(\mathscr{S}_6)^{\downarrow}\mathscr{O}$ subduced irreps for sixfold spin clusters pertaining to the molecular cage ion, $[^{11}BH]_6^{2-}$, Chem. Phys. 154 (1991) 97–110., J.P. Colpa and F.P. Temme 156 (1991) 532

Molecular interactions
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71
New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v)+NH_3 \rightarrow NH_2+NH_4^+$, A. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79
Pressure dependence of the polarized reflectance spectrum of a solid charge-transfer complex, perylene-hexacyanobutadiene (HCBD), T. Ida, K. Yakushi, H. Kuroda, H. Yamochi and G. Saito 156 (1991) 113
Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223
Electronic spectra and proton transfer in the phenol/$(NH_3)_n$ clusters in argon matrices, C. Crépin and A. Tramer 156 (1991) 281
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479

Spectral bandshapes and intensities
Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21

Theoretical study of multiple-scattering effects in the X-ray absorption spectra of iron-porphyrins, F. Bohr and M.F. Ruiz-López 156 (1991) 55
Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465
Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473
Optothermal-detected microwave-sideband CO_2-laser spectroscopy of NCH–NH_3, G.T. Fraser, A.S. Pine, W.A. Kreiner and R.D. Suenram 156 (1991) 523

Coupling of electronic and nuclear motion
Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21

Energy transfer processes
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123
Vibrational relaxation of glyoxal in collisions with He and Ar, G.-J. Kroes and R.P.H. Rettschnick 156 (1991) 293
Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339
State-to-state cross sections for rotational excitation of ortho- and para-NH_3 by He and H_2, J. Schleipen and J.J. ter Meulen 156 (1991) 479
Laser excitation of the $A^3\Sigma_u^+$, $A'^3\Delta_u$ and $c^1\Sigma_u^-$ states of molecular oxygen, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 156 (1991) 497

Molecular photophysical processes
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177
Vibrational and rotational effects on the intersystem crossing in pyrazine and pyrimidine, P. Uijt de Haag and W.L. Meerts 156 (1991) 197
Isomer-specific radiative lifetimes of molecular heteroclusters, D. Bahatt, U. Even, E. Shalev, N. Ben-Horin and J. Jortner 156 (1991) 223

Intramolecular dynamics
Real-time dynamics of vibrational predissociation in anthracene–Ar_n ($n=1,2,3$), A. Heikal, L. Bañares, D.H. Semmes and A.H. Zewail 156 (1991) 231
Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309

–radiationless transitions
S_1–T_1 coupling in propynal by level anticrossing spectroscopy, M. Lombardi, J.P. Pique, U. Brühlmann and J.R. Huber 156 (1991) 163
Energy and rotational state dependence of radiationless processes in propynal, P.R. Willmott, H. Bitto and J.R. Huber 156 (1991) 177

Luminescence spectra, yields and lifetimes
Magnetic field dependence of rotationally resolved excitation spectra of the $^1B_{3u}$ 0_0^0 transition of jet-cooled pyrazine, P.J. de Lange, H.Th. Jonkman and K.E. Drabe 156 (1991) 209

Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339

Non-linear responses (including optical)
Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism, K.D. Schulze 156 (1991) 43
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103

Multiphoton phenomena
Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509

Reactions (including dissociation)

–gas phase
New mechanism for the vibrational mode-specific proton-transfer reaction $NH_3^+(v) + NH_3 \rightarrow NH_2 + NH_4^+$. Tachibana, T. Suzuki, N. Yoshida, Y. Teramoto and T. Yamabe 156 (1991) 79
Dissociation of aliphatic hydrocarbons excited by electrons: translational energy distributions of the excited hydrogen atom, T. Ogawa, T. Tsuboi and K. Nakashima 156 (1991) 465
Dissociation of hydrogen sulfide in e–H_2S collisions: translational energy distribution of $H^*(n=4)$, T. Ogawa, M. Tsukada and K. Nakashima 156 (1991) 473

–condensed phase
Laser-initiated chain reactions and microexplosions in solid solutions of methylcyclopropane and chlorine, T.J. Tague Jr. and C.A. Wight 156 (1991) 141
Theory of diffusion-influenced fluorescence quenching: dependence of the Stern–Volmer curve on light intensity, S. Lee, M. Yang, K.J. Shin, K.Y. Choo and D. Lee 156 (1991) 339

Electron transfer
Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1

Ionization (including Rydberg states)
Localization and correlation corrections in electronic interactions through single bonded hydrocarbon spacers, M. Braga, A. Broo and S. Larsson 156 (1991) 1
Vibronic coupling in Rydberg series of linear molecules, A. Staib, W. Domcke and A.L. Sobolewski 156 (1991) 21
Many-body calculations of the core hole spectra of NiCO, M. Ohno and P. Decleva 156 (1991) 309
Theoretical study of optical excitations of linear C_4^-, L. Adamowicz 156 (1991) 387
Zeeman effect in the two-photon excitation spectrum of the $C^2\Pi$ state of NO, S. Guizard, N. Shafizadeh, D. Chapoulard, M. Horani and D. Gauyacq 156 (1991) 509

Molecular motion (including diffusive)
The trans-stilbene–Ar van der Waals complex. Vibrationally averaged substitution structure in its S_0 and S_1 electronic states, B.B. Champagne, D.F. Plusquellic, J.F. Pfanstiel, D.W. Pratt, W.M. van Herpen and W.L. Meerts 156 (1991) 251

Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid, A. Chandra and B. Bagchi 156 (1991) 323
Intramolecular dynamics of the C_4H_8NH radical cation. An application of the anisotropic exchange theory for powder ESR lineshapes, L. Sjöqvist, N.P. Benetis, A. Lund and J. Maruani 156 (1991) 457

Collective motion and excitations
Molecular dynamics simulation of crystalline imidazole, S. Besnainou, G. Cardini and D.A. Dows 156 (1991) 71
Electronic spectra of 4-nitro-pyridine-*n*-oxide (NPO) single crystals, M. Pierre, P.L. Baldeck, D. Block, R. Georges, H.P. Trommsdorff and J. Zyss 156 (1991) 103
Fluorescence depolarization in nonlinear molecular pairs, D. Gülen 156 (1991) 123
Effects of solvent viscoelasticity in the solvation dynamics of an ion in a dense dipolar liquid, A. Chandra and B. Bagchi 156 (1991) 323

Surface effects and catalysis
The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63
A theoretical study of the chemisorption of methane on a Ni(100) surface, O. Swang, K. Faegri Jr., O. Gropen, U. Wahlgren and P. Siegbahn 156 (1991) 379

Thermodynamic and transport properties
Scaling the WCA reference system for two-dimensional Lennard-Jones fluids, F. Cuadros and A. Mulero 156 (1991) 33

Structure of solids and liquids
On the elastic properties of lithium, sodium and potassium oxide. An ab initio study, R. Dovesi, C. Roetti, C. Freyria-Fava, M. Prencipe and V.R. Saunders 156 (1991) 11
Zinc ion in water: intermolecular potential with approximate three-body correction and Monte Carlo simulation, Y.P. Yongyai, S. Kokpol and B.M. Rode 156 (1991) 403

Critical phenomena
The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63

Phase transitions
Simulation of the unstable dynamics of excitable biomembranes: properties of a cyclic electrochemical gating mechanism, K.D. Schulze 156 (1991) 43
The influence of physisorption and the Eley–Rideal mechanism on a surface reaction: $CO+O_2$, J. Mai and W. von Niessen 156 (1991) 63